code: https://github.com/anandpratap/flame_1d

I. INTRODUCTION

The governing equations are,

$$\dot{m}\frac{\partial T}{\partial x} = \frac{\partial}{\partial x}\left(\alpha\frac{\partial T}{\partial x}\right) + \dot{\omega}_T(\mathbf{Y}, T) \tag{1}$$

$$\dot{m}\frac{\partial Y_k}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial Y_k}{\partial x}\right) + \ddot{\omega}_{Y_k}(\mathbf{Y}, T) \tag{2}$$

$$\tag{3}$$

Density is assumed to be constant (=1). The diffusivisty are assumed to be constant, $\alpha = D = 1.5 \times 10^{-5}$. Auxillary relations for the calculation of the source terms are,

$$\ddot{\omega}_{Y_k}(\mathbf{Y}, T) = \sum_{reactions} W_k \dot{\omega}_k \tag{4}$$

$$\dot{\omega}_T(\mathbf{Y}, T) = \sum_{reactions} \frac{1}{C_p} \sum_k \ddot{\omega}_{Y_k} h_k \tag{5}$$

$$\dot{\omega}_T(\mathbf{Y}, T) = \frac{Qq}{C_p}\text{(for the base case used for demo, as the above expression will lead to zero source)} \tag{6}$$

$$q = k_f \prod_k [X_k]^{\nu_{lhs,k}} - k_b \prod_k [X_k]^{\nu_{rhs,k}} \tag{7}$$

$$X_k = \frac{Y_k/W_k}{\sum_j Y_j/W_j} \tag{8}$$

$$\dot{\omega}_k = \left(\nu_{rhs,k} - \nu_{lhs,k}\right) q \tag{9}$$

The initial conditions should be carefully choosen as the solution depends on them.